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Title: Bounding the 239Pu(n,f) cross-section

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Bounding the ^{239}Pu(n,f) cross-section

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Thank you to Denise and Diane for guidance and to Fredrik, Morgan, and Kyle for input on the project. Funded by JA4X.

Introduction-Goal

GOAL: Bounding the neutron-induced ^{239}Pu fission cross section (n,f), ^{239}Pu(n,f), for 50 keV to 20 MeV

Introduction-Reaching the Goal

GOAL: Bounding the neutron-induced ^{239}Pu fission cross section (n,f), ^{239}Pu(n,f), for 50 keV to 20 MeV

Aims towards this goal:

- Extract all ^{239}Pu(n,f) experimental data entering the current evaluation
- Choose data sets likely to influence the evaluation.
- Investigate which uncertainty sources are expected for these observables and develop an algorithm to estimate total covariances.
- Investigate whether uncertainties of chosen data sets are reasonable and update them.
- Mentor will re-evaluate with new information.

Introduction-Current Evaluation

- The current ^{239}**Pu(n,f) evaluation** is **provided by the neutron-cross section standards project** coordinated by the IAEA. (https://www-nds.iaea.org/standards/)

- **using the "GMA" code and database with a Generalized Least Squares algorithm**. Poenitz, ANL/NDM-139 (1997):

$$\delta = (A^T C_M^{-1} A)^{-1} A^T C_M^{-1} M$$

where δ is the adjustment vector, **A** is the coefficient matrix, **C** is the correlation matrix of the measurement vector **M**, superscript T denotes the transpose, and -1 the inverse matrices. The variance-covariance matrix of δ follows from error propagation:

$$C_\delta = (A^T C_M^{-1} A)^{-1}.$$

- GMA database contains data of the following reactions: ^{6}Li(n,α), ^{10}B(n,$\alpha_{(1)}$), Au(n,γ), ^{235}U(n,f), ^{238}U(n,f), ^{238}U(n,γ), ^{239}Pu(n,f), averaged Cf fission spectrum

Extract all ^{239}Pu(n,f) experimental data entering the current evaluation

Data bases we Investigated

“Standards Report”

- gave a list of ^{239}Pu(n,f) cross section data sets in Table 7.1 of IAEA Report STI/PUB/1291 (2007).

EXFOR

- extracted these data sets and partial uncertainties from EXFOR (https://www-nds.iaea.org/exfor/exfor.htm) and an EXFOR-like library provided by R. Capote on 5/25/2017 in private communication.

GMA

- extracted total uncertainties for each data set from GMA output file provided by R. Capote on 5/12/2017 in private communication.

Data Types

Absolute: $^{239}Pu(n,f)$ cross section measured over its given energy range including the normalization

Shape: $^{239}Pu(n,f)$ cross section without a set normalization

Data Types

Clean Ratio Absolute: ^{239}Pu(n,f) cross section measured in ratio to a reference isotope in the same fission detector

Clean Ratio Shape: Clean Ratio Data without a set normalization

Examples: ^{239}Pu(n,f)/^{235}U(n,f), ^{239}Pu(n,f)/^{238}U(n,f)

Data Types

Indirect Ratio Absolute: $^{239}Pu(n,f)$ cross section measured in ratio to a reference isotope, which is measured in a different detector

Indirect Ratio Shape: Indirect Ratio Data without a set normalization

Examples: $^{239}Pu(n,f)/^{10}B(n,\alpha)$, $^{239}Pu(n,f)/^{6}Li(n,\alpha)$

Statistics on Extracted Data

Data Type	Absolute	Shape	Clean Ratio Absolute	Clean Ratio Shape	Indirect Ratio Absolute	Clean Ratio Shape
Number of Data Sets	16	3	17 (16 relative to $^{235}U(n,f)$, 1 relative to $^{238}U(n,f)$)	6 (4 relative to $^{235}U(n,f)$, 2 relative to $^{238}U(n,f)$)	0	19 (17 relative to $^{10}B(n,\alpha)$, 2 relative to $^{6}Li(n,\alpha)$)

Choose data sets likely to influence the evaluation

Choosing the Data Sets

Criteria:

- Energies above 50 keV
- Low Total Uncertainties Compared to Other Data Sets
- Broad Energy Range
- Calibration Point
- Missing Partial Uncertainties in EXFOR entry

Choosing the Data Sets

Data Set	Data Type	Min δ	Max δ	Min E	Max E	EXFOR #
611	absolute	1.0	1.0	1.45E+01	1.45E+01	
644	absolute	2.0	2.0	1.45E+01	1.45E+01	30634
615	absolute	2.1	2.1	5.00E+00	5.00E+00	
1038	absolute	2.3	7.7	1.00E+00	5.50E+00	30670
640	absolute	2.4	3.1	1.50E-01	9.60E-01	10314
620	absolute	2.8	6.6	3.00E-02	9.80E-01	20567
⋮						
8002	ratio absolute ^{235}U(n,f)	0.7	3.8	2.00E-01	1.30E+01	14271
602	ratio absolute ^{235}U(n,f)	0.8	6.8	2.53E-08	1.00E+01	
654	ratio absolute ^{235}U(n,f)	1.0	5.7	2.40E-02	7.50E+00	
685	ratio absolute ^{235}U(n,f)	1.1	1.1	1.45E+01	1.45E+01	
653	ratio absolute ^{235}U(n,f)	1.2	6.9	1.20E-01	7.00E+00	40824
1014	ratio absolute ^{235}U(n,f)	1.3	1.6	8.50E-01	6.00E+01	13801
600	ratio absolute ^{235}U(n,f)	1.7	27.4	8.50E-04	3.00E+01	10562
605	ratio absolute ^{235}U(n,f)	1.7	15.3	5.50E-03	1.00E+00	20363
608	ratio absolute ^{235}U(n,f)	2.0	12.6	4.50E-02	5.00E-01	21463
609	ratio absolute ^{235}U(n,f)	2.0	2.1	1.00E+00	1.40E+01	21195
631	ratio absolute ^{235}U(n,f)	2.1	2.1	2.53E-08	1.50E-01	
1012	ratio absolute ^{235}U(n,f)	2.1	5.8	5.70E-01	2.00E+02	41455
⋮						
630	ratio shape ^{10}B(n,α)	2.3	5.0	2.53E-08	1.50E-01	
⋮						
535	ratio shape ^{6}Li(n,α)	2.3	4.1	1.50E-04	9.50E-02	
536	ratio shape ^{235}U(n,f)	0.7	6.5	2.53E-08	2.10E+01	12766
1029	ratio shape ^{235}U(n,f)	1	2.5	5.00E-01	2.00E+02	
549	ratio shape ^{235}U(n,f)	2.0	3.6	1.50E-04	1.50E-02	
635	ratio shape ^{235}U(n,f)	3.1	123.1	2.53E-08	2.40E-02	10084
837	ratio shape ^{238}U(n,f)	2.6	3.7	1.30E+01	1.90E+01	
407	ratio shape ^{238}U(n,f)	3.7	6.3	4.00E-01	1.40E+00	
521	shape	2.3	4.8	1.00E+00	2.10E+01	20786

Investigate which uncertainty sources are expected for these observables and develop an algorithm to estimate total covariances.

Sources of Uncertainty

Absolute Data

Attenuation
Background Determination
Correction for Isotopic Impurities in the Sample
Detector Efficiency
Energy Resolution
Fission Fragment Angular Distribution Correction
Multiple Scattering
Neutron Flux
Sample Mass
Statistics
Time of Flight Length

Sources of Uncertainty

Shape Data

Attenuation
Background Determination
Correction for Isotopic Impurities in the Sample
Detector Efficiency
Energy Resolution
Fission Fragment Angular Distribution Correction
Multiple Scattering
Neutron Flux
Sample Mass
Statistics
Time of Flight Length

Sources of Uncertainty

Clean Ratio Absolute Data

^{239}Pu(n,f)

Correction for Isotopic Impurities

Detector Efficiency

Sample Mass

Reference Isotope

Correction for Isotopic Impurities

Detector Efficiency

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Combined

Attenuation

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Sources of Uncertainty

Clean Ratio Shape Data

^{239}Pu(n,f)

Correction for Isotopic Impurities

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Correction for Isotopic Impurities

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Time of Flight Length

Sources of Uncertainty

Indirect Ratio Absolute Data

^{239}Pu(n,f)

- Angular Correction
- Attenuation
- Background Determination
- Correction for Isotopic Impurities
- Detector Efficiency
- Energy Resolution
- Multiple Scattering
- Sample Mass
- Time of Flight Length

Reference Isotope

- Angular Correction
- Attenuation
- Background Determination
- Correction for Isotopic Impurities
- Detector Efficiency
- Energy Resolution
- Multiple Scattering
- Sample Mass
- Time of Flight Length

Combined

- **Neutron Flux**
- Statistics

Sources of Uncertainty

Indirect Ratio Shape Data

^{239}Pu(n,f)

Angular Correction
Attenuation
Background Determination
Correction for Isotopic Impurities
Detector Efficiency
Energy Resolution
Multiple Scattering
Sample Mass
Time of Flight Length

Reference Isotope

Angular Correction
Attenuation
Background Determination
Correction for Isotopic Impurities
Detector Efficiency
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Sample Mass
Time of Flight Length

Combined

Neutron Flux
Statistics

Covariance Algorithm

Example: Shape Measurement

E_i	i^{th} energy bin
n	set normalization
σ	absolute cross section
ξ	shape measurement

ABSOLUTE CROSS SECTION

$$\sigma(E_i) = n\xi(E_i)$$

LINEAR ERROR PROPAGATION

$$Cov(\sigma_i, \sigma_j) = \left.\frac{\partial \sigma}{\partial n}\right|_{E_i} (\Delta n)^2 \left.\frac{\partial \sigma}{\partial n}\right|_{E_j} + \left.\frac{\partial \sigma}{\partial \xi}\right|_{E_i} Cov(\xi_i, \xi_j) \left.\frac{\partial \sigma}{\partial \xi}\right|_{E_j}$$

Covariance Algorithm

Example: Shape Measurement

$$
\begin{aligned}
Cov(\xi_i, \xi_j) = {} & \Delta b_i \Delta b_j Cor(b_i, b_j) \\
& + \Delta\alpha_i \Delta\alpha_j Cor(\alpha_i, \alpha_j) \\
& + \Delta\beta_i \Delta\beta_j Cor(\beta_i, \beta_j) \\
& + \Delta\epsilon_i \Delta\epsilon_j Cor(\epsilon_i, \epsilon_j) \\
& + \Delta c_i \Delta c_j \delta_{ij} \\
& + \Delta\zeta_i \Delta\zeta_j Cor(\zeta_i, \zeta_j) \\
& + \left.\frac{\partial\xi}{\partial E_i}\right|_{E_i} \Delta E_i \Delta E_j Cor(E_i, E_j) \left.\frac{\partial\xi}{\partial E_j}\right|_{E_j}
\end{aligned}
$$

Investigate whether uncertainties of chosen data sets are reasonable and update them.

Total Uncertainty Ranges

Data Set	Data Type	Min δ	Max δ	Min E	Max E	EXFOR #
611	absolute	1.0	1.0	1.45E+01	1.45E+01	
644	absolute	2.0	2.0	1.45E+01	1.45E+01	30634
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685	ratio absolute ^{235}U(n,f)	1.1	1.1	1.45E+01	1.45E+01	
653	ratio absolute ^{235}U(n,f)	1.2	6.9	1.20E-01	7.00E+00	40824
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549	ratio shape ^{235}U(n,f)	2.0	3.6	1.50E-04	1.50E-02	
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Uncertainty Ranges found in EXFOR for Absolute Data

Data Sets	611	1038	620
Uncertainty Data Types	E,CS,C	CS,C	E,CS,C
P1		1.5	1.0
P2	0.3 - 0.3	0.9 - 1.8	1.5 - 1.8
P3	0.36		0.5 - 0.70
P4	1.04	1.47	1.84 - 1.94
P5			1.0 - 1.0
P6		1.15 - 1.5	0.8 - 1.0
P7	0.3		
P8	1.01 - 1.01		2.82 - 26.3
P9			
P10		5.0	0.5 - 0.5
P11			

P1 - Sample Mass
P2 - Statistics
P3 - Attenuation
P4 – Detector Efficiency
P5 - Fission Fragment Angular Distribution Correction

P6 - Background Determination
P7 - Time of Flight Length Uncertainty
P8 - Energy Resolution
P9 - Neutron Flux
P10 - Multiple Scattering
P11 - Correction for Isotopic Impurities

Updated Uncertainty Ranges

Data Sets	611	1038	620
Uncertainty Data Types	E,CS,C	CS,C	E,CS,C
P1	1.0	1.5	1.0
P2	0.3 - 0.3	0.9 - 1.8	1.5 - 1.8
P3	0.36	ok	0.5 - 0.70
P4	1.04	1.47	1.84 - 1.94
P5	ok	ok	1.0 - 1.0
P6	0.5	1.15 - 1.5	0.8 - 1.0
P7	0.3	ok	ok
P8	1.01 - 1.01	?	2.82 - 26.3
P9	?	ok	?
P10	ok	5.0	0.5 - 0.5
P11	ok	ok	ok

P1 - Sample Mass

P2 - Statistics

P3 - Attenuation

P4 – Detector Efficiency

P5 - Fission Fragment Angular Distribution Correction

P6 - Background Determination

P7 - Time of Flight Length Uncertainty

P8 - Energy Resolution

P9 - Neutron Flux

P10 - Multiple Scattering

P11 - Correction for Isotopic Impurities

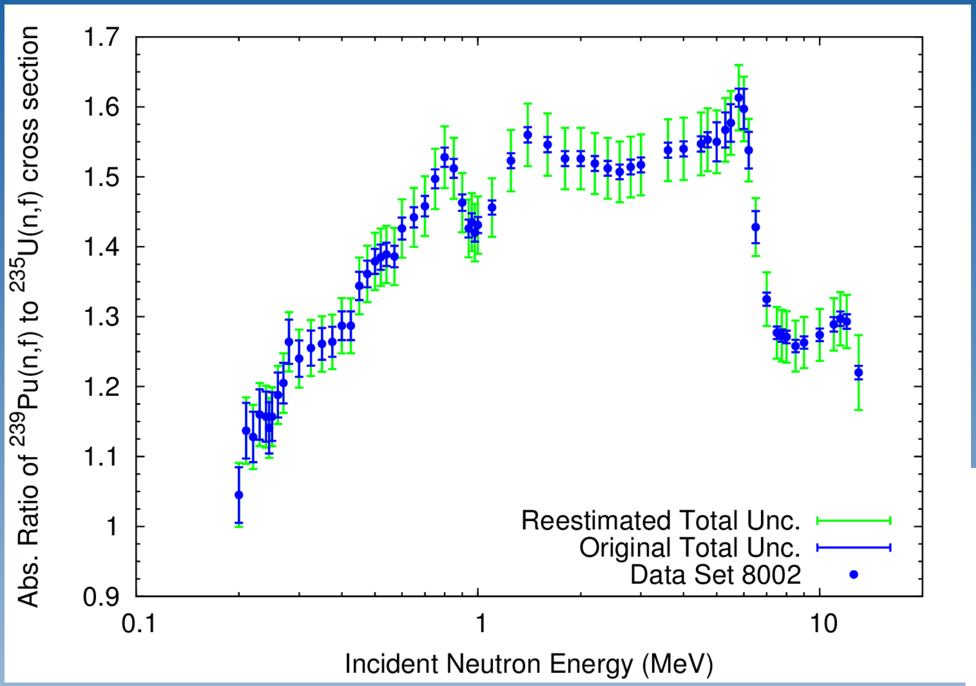
Uncertainty Ranges Found in EXFOR for Ratio Data

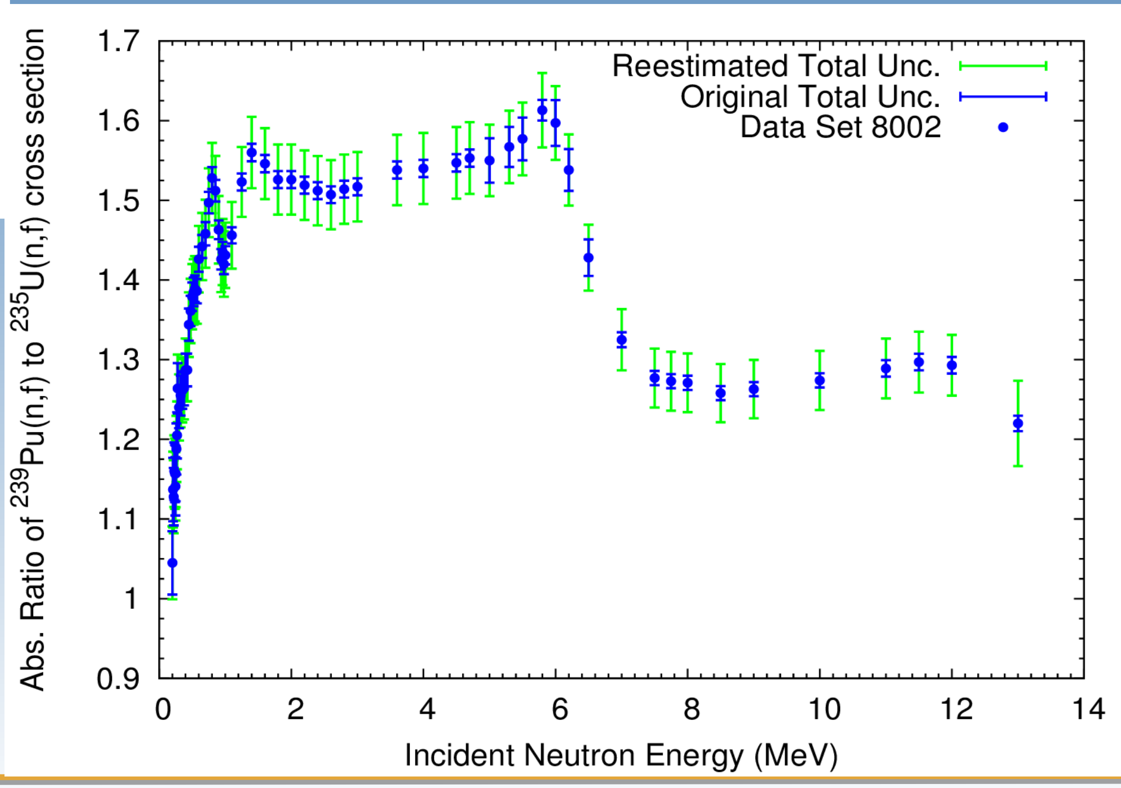
Data Sets	8002	602	685	630	535	536	1029
Uncertainty Data Types	CS,C	E,CS,C	E,CS,C	E,CS	E,CS	E,CS	CS,C
P1		0.63 - 1.99	0.94				0.94
P2	0.3 - 1.5			0.7 - 0.8	0.2 - 1.2	0.4 - 1.7	0.62 - 2.27
P3			0.2 - 0.2	1.0 - 1.0			
P4		0.2 - 0.2		0.5 - 0.5	3.16 - 4.07	0.3 - 0.3	
P5							
P6	0.4 - 3.2	0.1 - 0.7		1.0 - 1.0	0.1 - 0.2	0.3 - 0.3	
P7		0.3 - 2.22		5.0 - 5.0		1.0 - 1.0	
P8		0.0 - 21.7	1.0 - 1.0	5.0 - 5.0	0.1 - 33.3	1.0 - 1.0	
P9							
P10		0.2 - 0.3	0.2 - 0.2	1.0 - 1.0			
P11			0.2				
M1	2	0.63 - 1.99	0.94				0.99
M2	2		0.4 - 0.4	0.7 - 0.8	0.2 - 1.2	0.4 - 1.7	0.62 - 2.27
M3				1.0 - 1.0			
M4				1.0 - 1.0	3.0 - 3.7	0.3 - 0.3	
M5							
M6	0.3 - 3.1						
M10			0.2 - 0.2				
M11			0.3				

Updated Uncertainty Ranges

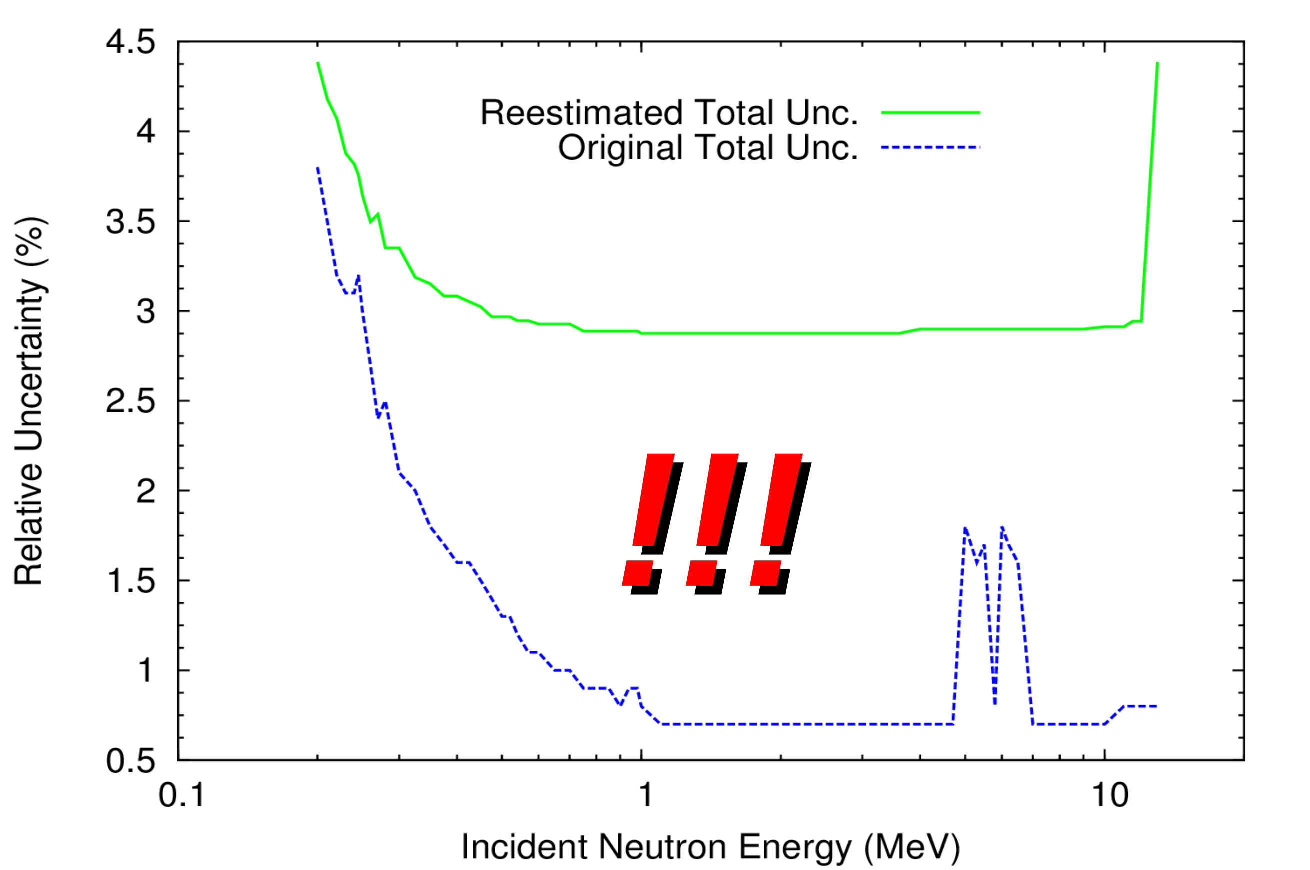
Data Sets	8002	602	685	630	535	536	1029
Uncertainty Data Types	CS,C	E,CS,C	E,CS,C	E,CS	E,CS	E,CS	CS,C
P1	2	0.63 - 1.99	0.94	ok	ok	ok	0.94
P2	0.3 - 1.5	?	?	0.7 - 0.8	0.2 - 1.2	0.4 - 1.7	0.62 - 2.27
P3	ok	ok	0.2 - 0.2	1.0 - 1.0	?	?	ok
P4	ok	0.2 - 0.2	ok	0.5 - 0.5	3.16 - 4.07	0.3 - 0.3	ok
P5	ok	ok	ok	?	?	?	ok
P6	0.4 - 3.2	0.1 - 0.7	?	1.0 - 1.0	0.1 - 0.2 ?	0.3 - 0.3	0.4-3.2
P7	3mm	0.3 - 2.22	ok	5.0 - 5.0	ok	1.0 - 1.0	3mm
P8	ok	0.0 - 21.7	1.0 - 1.0	5.0 - 5.0	0.1 - 33.3	1.0 - 1.0	ok
P9	ok	ok	ok	ok	ok	ok	ok
P10	ok	0.2 - 0.3	0.2 - 0.2	1.0 - 1.0	?	ok	ok
P11	ok	ok	0.2	ok	ok	ok	ok
M1	~~2~~	0.63 - 1.99	0.94	ok	ok	ok	0.99
M2	~~2~~	?	0.4 - 0.4 ok	0.7 - 0.8	0.2 - 1.2	0.4 - 1.7	0.62 - 2.27
M3	ok	ok		1.0 - 1.0			ok
M4	ok	ok	ok	1.0 - 1.0	3.0 - 3.7	0.3 - 0.3	ok
M5	ok	ok	ok	ok	ok	ok	ok
M6	0.3 - 3.1	ok	ok	ok	?	ok	0.3-3.1
M10	ok	ok	0.2 - 0.2	ok	?	ok	ok
M11	?	?	0.3	?	?	?	?

Example: Tovesson Data Set





Example: Tovesson Data Set



Summary

GOAL: Bounding the neutron-induced ^{239}Pu fission cross section (n,f), ^{239}Pu(n,f), for 50 keV to 20 MeV

<u>Aims towards this goal:</u>

- ✓ Extract all ^{239}Pu(n,f) experimental data entering the current evaluation
- ✓ Choose data sets likely to influence the evaluation.
- ✓ Investigate which uncertainty sources are expected for these observables and develop algorithm to estimate total covariances.
- ✓ Investigate whether uncertainties of chosen data sets are reasonable and update them.

To-Do Mentor

- GMA studies to see how these changes affect the evaluated uncertainties
- GMA studies on missing cross-correlations between experimental data.
- See if the thermal $^{239}Pu(n,f)$ cross-section has an impact.

Thank you for your attention

Back Up Slides

Table of Selected Data Sets

Data Set	Data Type	Min δ	Max δ	Min E	Max E	EXFOR #
611	absolute	1.0	1.0	1.45E+01	1.45E+01	
644	absolute	2.0	2.0	1.45E+01	1.45E+01	30634
615	absolute	2.1	2.1	5.00E+00	5.00E+00	
1038	absolute	2.3	7.7	1.00E+00	5.50E+00	30670
640	absolute	2.4	3.1	1.50E-01	9.60E-01	10314
620	absolute	2.8	6.6	3.00E-02	9.80E-01	20567
622	absolute	2.8	7.0	8.00E-01	2.60E+00	20570
619	absolute	2.9	2.9	2.40E-02	2.40E-02	20584
621	absolute	2.9	3.2	9.50E-03	2.00E-01	20569
623	absolute	3.2	4.1	2.60E+00	5.50E+00	20618
612	absolute	3.8	5.7	1.40E+01	1.45E+01	20779
672	absolute	4.9	5.4	5.40E-01	1.60E+00	
616	absolute	5.4	5.4	1.90E+01	1.90E+01	
617	absolute	5.8	5.8	8.50E+00	8.50E+00	
628	absolute	5.9	5.9	1.40E+01	1.40E+01	21468
657	absolute	9.3	9.3	1.40E+01	1.40E+01	
8002	ratio absolute ^{235}U(n,f)	0.7	3.8	2.00E-01	1.30E+01	14271
602	ratio absolute ^{235}U(n,f)	0.8	6.8	2.53E-08	1.00E+01	
654	ratio absolute ^{235}U(n,f)	1.0	5.7	2.40E-02	7.50E+00	
685	ratio absolute ^{235}U(n,f)	1.1	1.1	1.45E+01	1.45E+01	
653	ratio absolute ^{235}U(n,f)	1.2	6.9	1.20E-01	7.00E+00	40824
1014	ratio absolute ^{235}U(n,f)	1.3	1.6	8.50E-01	6.00E+01	13801
600	ratio absolute ^{235}U(n,f)	1.7	27.4	8.50E-04	3.00E+01	10562
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633	ratio absolute ^{235}U(n,f)	3.3	3.3	1.50E+01	1.50E+01	
666	ratio absolute ^{235}U(n,f)	5.7	6.2	1.40E+01	1.50E+01	30588
668	ratio absolute ^{238}U(n,f)	10.3	10.3	1.40E+01	1.40E+01	
1024	ratio shape ^{10}B(n,α)	0.8	4.6	1.50E-04	1.50E-02	
551	ratio shape ^{10}B(n,α)	1.5	7.3	2.53E-08	4.50E-02	40751
548	ratio shape ^{10}B(n,α)	1.7	9.6	1.50E-04	2.40E-02	
719	ratio shape ^{10}B(n,α)	2.2	15.6	1.50E-04	2.40E-02	20001
630	ratio shape ^{10}B(n,α)	2.3	5.0	2.53E-08	1.50E-01	
677	ratio shape ^{10}B(n,α)	3.0	5.7	1.50E-04	9.50E-03	
676	ratio shape ^{10}B(n,α)	3.4	32.6	2.53E-08	1.50E-01	
679	ratio shape ^{10}B(n,α)	3.7	20.1	1.50E-04	1.50E-02	
680	ratio shape ^{10}B(n,α)	3.7	4.2	1.50E-04	2.40E-02	
681	ratio shape ^{10}B(n,α)	3.7	8.2	2.53E-08	1.50E-02	
682	ratio shape ^{10}B(n,α)	3.7	10.0	2.53E-08	1.50E-02	
678	ratio shape ^{10}B(n,α)	4.7	31.6	1.50E-04	9.50E-03	
662	ratio shape ^{10}B(n,α)	5.4	11.9	1.50E-04	9.50E-03	

Table of Selected Data Sets

663	ratio shape ^{10}B(n,α)	5.4	15.6	1.50E-04	3.00E-02	
661	ratio shape ^{10}B(n,α)	6.4	7.7	1.50E-04	9.50E-02	
660	ratio shape ^{10}B(n,α)	7.1	7.5	1.50E-04	9.50E-02	
547	ratio shape ^{10}Li(n,α)	1.5	5.1	2.53E-08	4.50E-03	
535	ratio shape ^{10}Li(n,α)	2.3	4.1	1.50E-04	9.50E-02	
536	ratio shape ^{235}U(n,f)	0.7	6.5	2.53E-08	2.10E+01	12766
549	ratio shape ^{235}U(n,f)	2.0	3.6	1.50E-04	1.50E-02	
635	ratio shape ^{235}U(n,f)	3.1	123.1	2.53E-08	2.40E-02	10084
837	ratio shape ^{238}U(n,f)	2.6	3.7	1.30E+01	1.90E+01	
407	ratio shape ^{238}U(n,f)	3.7	6.3	4.00E-01	1.40E+00	
521	shape	2.3	4.8	1.00E+00	2.10E+01	20786
589	shape	2.9	3.9	1.50E-03	9.60E-01	20428
671	shape	4.3	25.8	3.00E-02	3.00E+00	21075